Principal Component Analysis (PCA)-based ROMs

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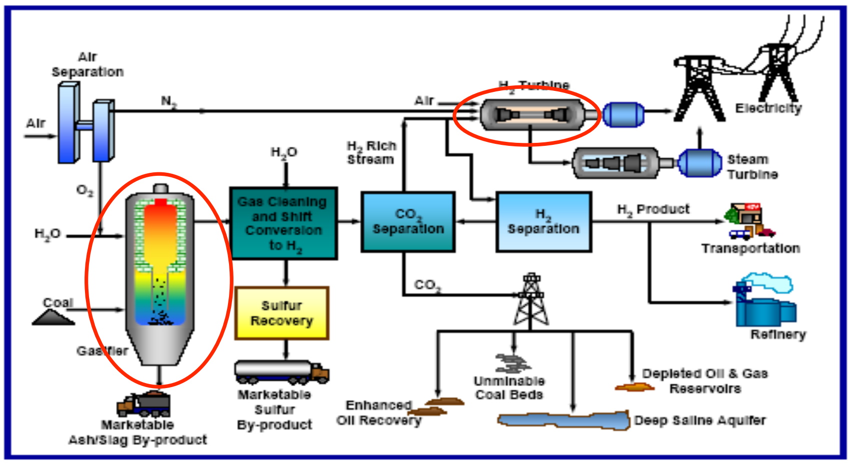
Outline

- Motivation
- Case Studies --- Combustor and Gasifier
- Background and Methodology of ROM Development
- Integration of ROM into Flowsheet Optimization
- Validation with Fluent
- Conclusions

Motivation

CFD model replaces Aspen Model → ROM replaces CFD Model



FutureGen Power Plant Flowsheet ---- Simulate closer to reality

Background of Models

- Geometry
- PDAE
- Flow pattern
- Energy Balance
- Chem. Reactions
- Properties
- 2,3-D

Complexity

Aspen + Fluent (APECS)

Steady State

PDE Model need not be reprocessed

Construct State Space Model independent of geometry

ROM on PCA

State Space Model

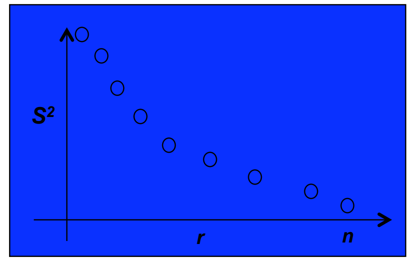
PCA and ROM based on PCA

Procedures of PCA

1. Singular Value Decomposition (SVD) $Y = USV^T$

2. Determine rank r: Cut-off criterion

$$R_r = \frac{\sum_{k=1}^{r} s_k^2}{\sum_{k=1}^{n} s_k^2} \le 1$$



3. Result of PCA

$$Y \approx Y_r = U_r S_r V_r^T = U_r C_r$$

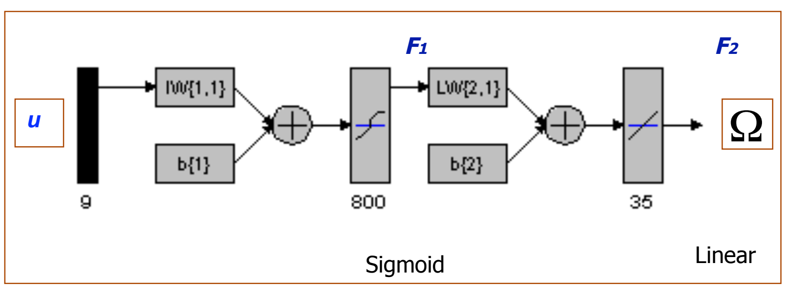
ROM Based on PCA

$$v(u): \{u_1, u_2, \cdots, u_k\} \mapsto C_r$$

$$\begin{bmatrix} x(u) \\ y(u) \end{bmatrix} = \begin{bmatrix} P & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} v(u) \\ w(u) \end{bmatrix} \cdot \mathbf{u}$$

How to do the mapping?

Mapping with Neural Network



$$\Omega = \begin{bmatrix} v(\mathbf{u}) \\ w(\mathbf{u}) \end{bmatrix} = F_2(LW\{1,1\} \cdot (F_1(IW\{2,1\} \cdot \mathbf{u} + b\{1\}) + b\{2\})$$

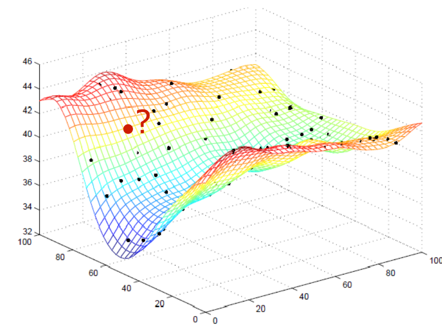
$$ROM: \quad \begin{bmatrix} x(u) \\ y(u) \end{bmatrix} = \begin{bmatrix} P & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} v(u) \\ w(u) \end{bmatrix} \cdot \mathbf{u}$$

"A network of two layers, where the first layer is sigmoid and the second layer is linear, can be trained to approximate any function arbitrarily well."

--- H. Demuth et al, "Neural Network Toolbox" (2005)

Mapping with Kriging

$$\Omega(u_i),\ i = 1,\ldots,m$$



$$\boxed{\Omega = \begin{bmatrix} v(\mathbf{u}) \\ w(\mathbf{u}) \end{bmatrix} = \sum_{i=1}^{n} f(u_i)\beta_i}$$

$$ROM: \quad \begin{bmatrix} x(u) \\ y(u) \end{bmatrix} = \begin{bmatrix} P & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} v(u) \\ w(u) \end{bmatrix} \cdot \mathbf{u}$$

Comparison of NNET & Kriging

Methods of Mapping

	Neural Network	Kriging
Uniqueness of Mapping	No.	Yes
CPUs of Model building	~1000-2000	<1
Sensitivity to # of Points	Higher.	Lower.
Accuracy of Approximation	No observable difference	

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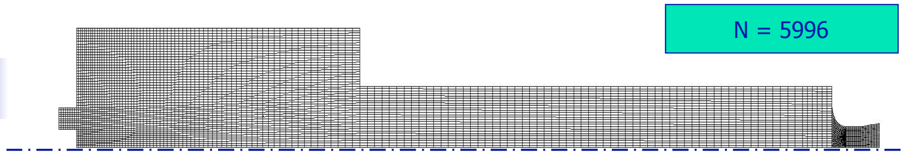
Case Study 1:

Gas turbine combustor

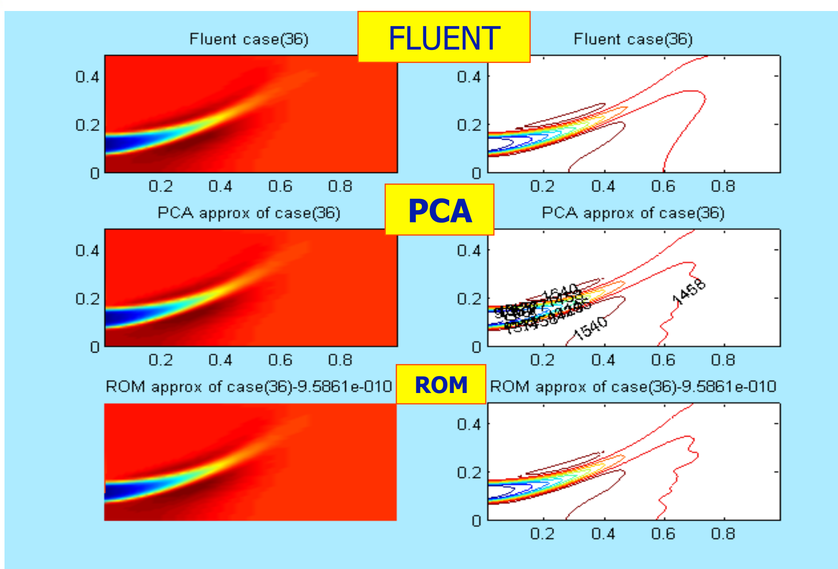
Geometry & mesh of the combustor



Typical temperature field in the combustor

Interest area of temperature field

Comparison of Results

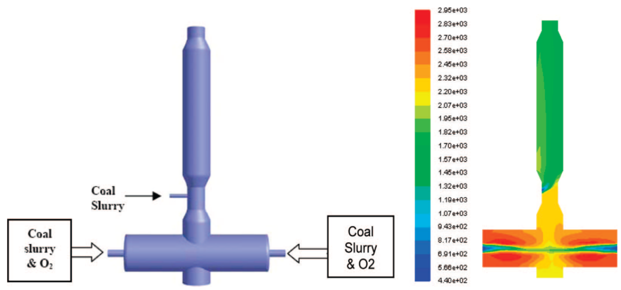


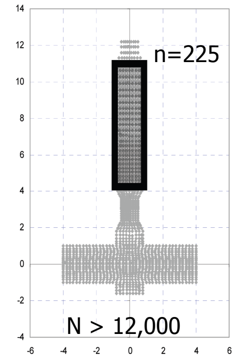
Average Fluent Case	~2000 CPU sec
Each case in ROM	< 1 CPU sec

Ranges of inputs of gasifier

Case Study 2 :

Entrained-Flow Coal Gasifier





Entrained-flow Gasifier, its typical temperature profile, meshed with Fluent and interest area

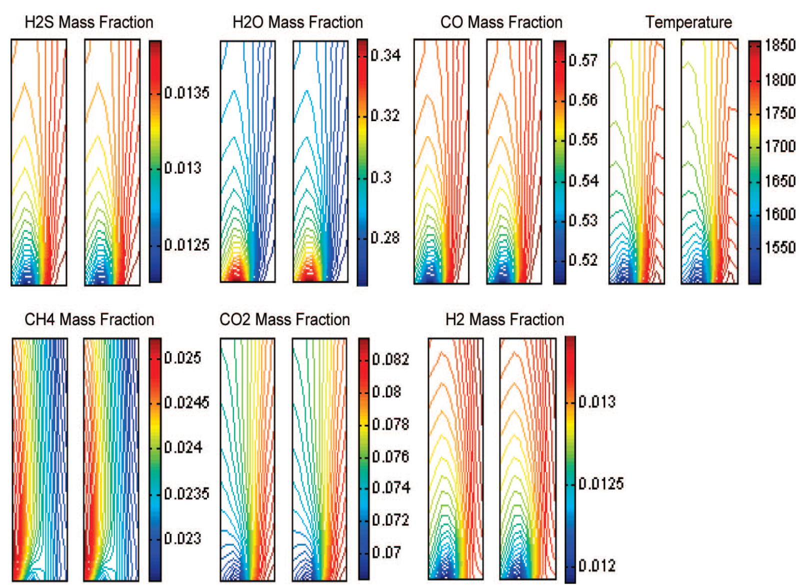
Operation Window of Gasifier

	Lower bound	Shi's value	Upper bound
u1	25	30	35
u2	0.75	0.817	0.85
u3	70	78	85

u1 --- the percentage of coal to inject between stage one and stage two;
u2 --- *the water percentage in the slurry;*
u3 --- the oxygen/coal feed ratio.

Comparison of Results

Contour plots of seven states



Average Fluent Case ~72 000 CPU sec

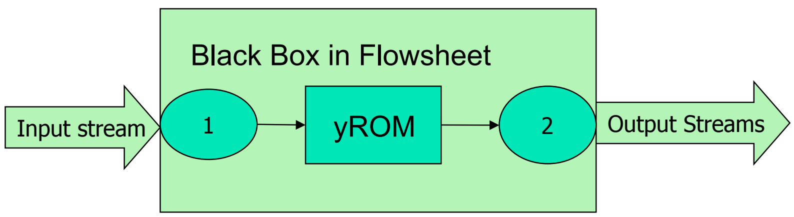
Each case in ROM < 1 CPU sec

Flowsheet Integration of ROM

Inputs	Outputs (s82)
u1 = Ratio of s84 to s83 [%]	Mass fraction of H2S
	Mass fraction of H2O
u2 = water in coal slurry [w/w %]	Mass fraction of H2
	Mass fraction of CH4
u3 = Ratio of oxygen to carbon [kmol/kmol %]	Mass fraction of CO2
	Mass fraction of CO
	Temperature [K]

- In flowsheet, inputs and outputs of model are states and component flowrates in streams.

- Integrating the ROM:
1. Convert boundary and operating conditions of yROM into input streams of model
2. Convert outputs of yROM into output streams of model



ROM Integration for Gasifier

Gasifier yROM becomes the Gasifier Flowsheet model

Inputs	Outputs (s82)
u1 = Ratio of s84 to s83 [%]	Mass fraction of H2S
	Mass fraction of H2O
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	Mass fraction of CO
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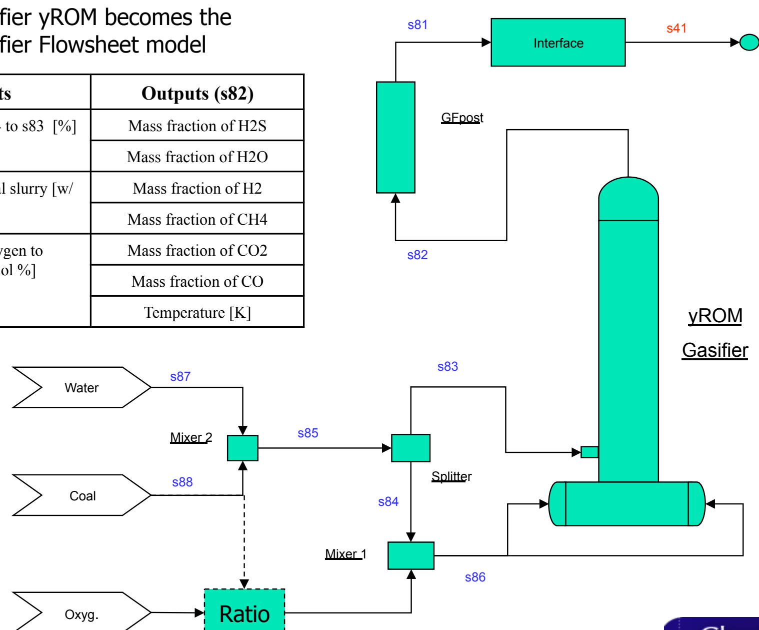
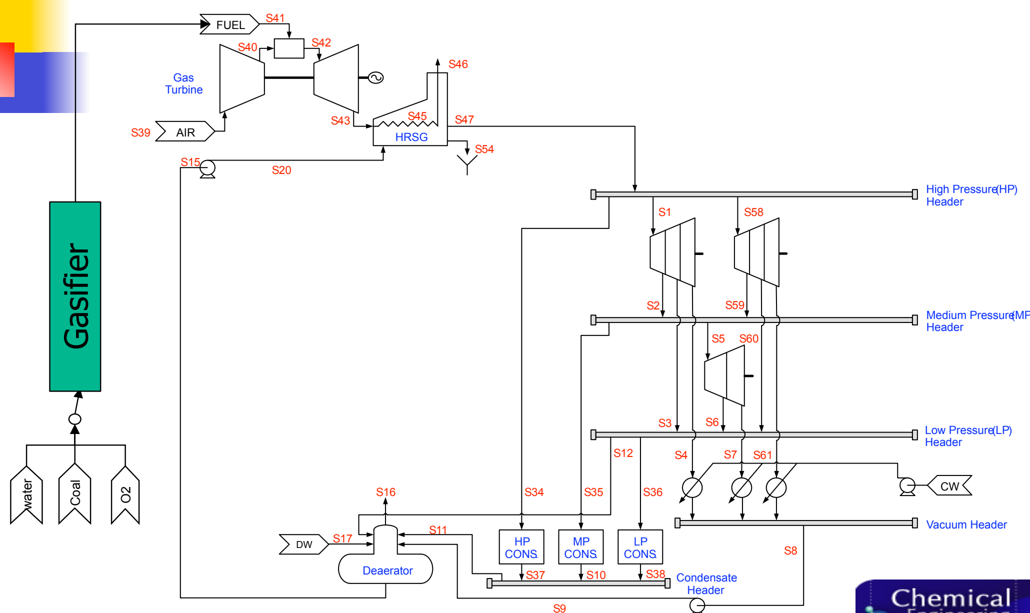


Integration of Gasifier ROM and Steam Cycle



Optimal Solution

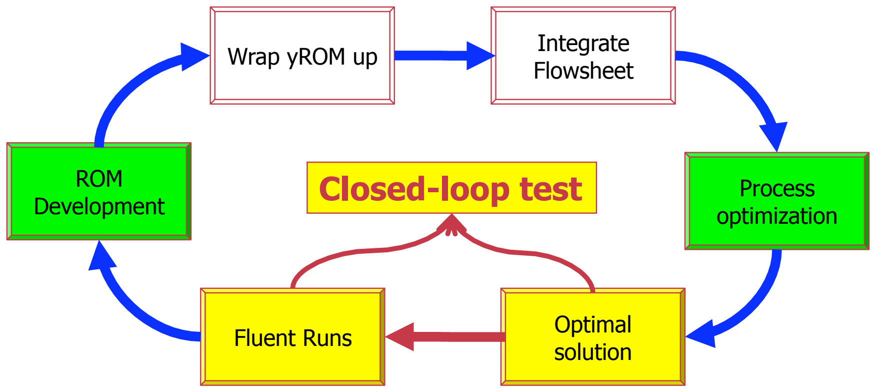
Minimizing Objective Function Subject to

Power Demand (Net Electricity): **500** MW

	Objective Function	Add. Constr	Optimal solutions		
			u1	u2	u3
1	Heating Value of Syngas	No	84.6928	34.9266	84.8813
2	Coal Feed flowrate	No	70.3411	25.2085	75.2154
3	Heating Value of Syngas	Tout >1660 Tout < 1670	84.6928	34.9266	82.716198
4	Coal Feed flowrate	Tout >1660 Tout < 1670	70.3411	25.2085	75.912813

Closing the Loop

Closed-loop Test: Run Fluent at the optimal solution, then test the consistency between the solution of Fluent and ROM predictions at the optimal solution



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Optimization Results ROM vs. CFD Model

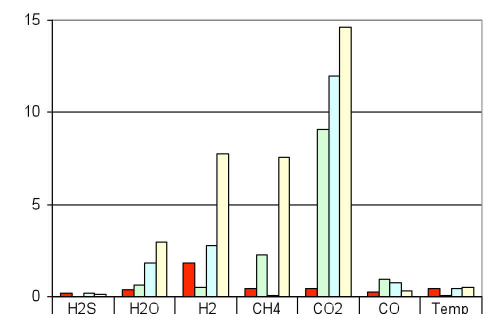
Fluent should converged with errors of

continuity 1.0e-6

energy 1.0e-6

do-intensi 1.0e-6

	Residuals		
	Continuity	Enegy	DO-intensity
Case 1	4.10E-06	6.45E-07	2.92E-05
Case 2	9.48E-06	1.09E-07	7.98E-05
Case 3	2.33E-04	4.10E-05	5.53E-04
Case 4	1.98E-04	6.82E-06	4.37E-04



	H2S	H2O	H2	CH4	CO2	CO	Temp
Case 1	0.20311	0.37995	1.84072	0.41165	0.44552	0.23151	0.41060
Case 2	0.02011	0.62983	0.48576	2.27500	9.08430	0.93594	0.03693
Case 3	0.17401	1.80365	2.76817	0.06850	11.9952	0.73518	0.45936
Case 4	0.09924	2.96652	7.73165	7.59190	14.6513	0.33569	0.48395

- For all four cases:

  Good Agreement for temperature, mass fractions of H2S, CO and H2O
  Good agreement of H2 and H2O for three cases;
  CO2 needs improvement for three cases - heavily dependent on Fluent resids.

- Effective and efficient ROM for process optimization

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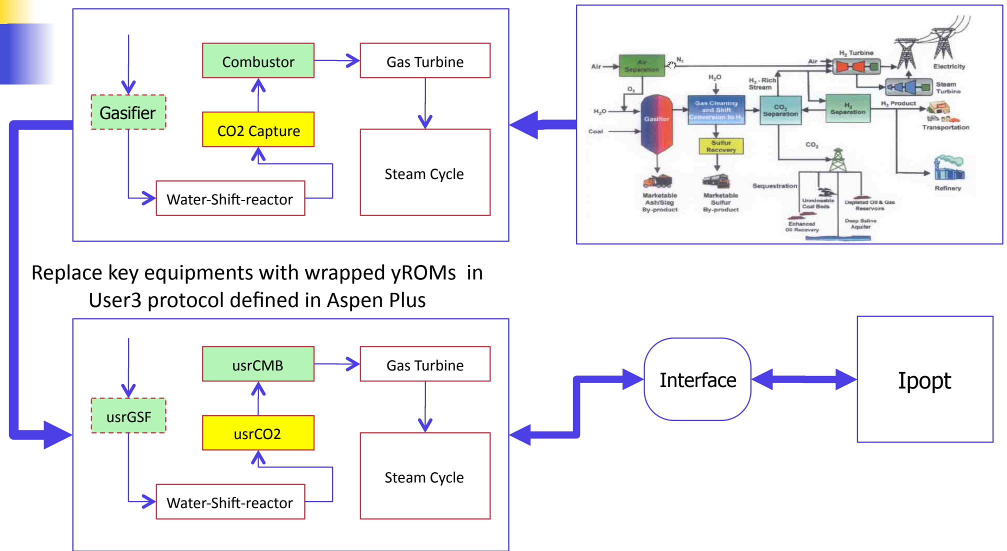
Current Work

Topology of Flowsheet of IGCC into Aspen Plus referring to TNO as a platform



Conclusions

- PCA-based ROM takes full advantage of commercial packages and retains the complexities of CFD
- No significant accuracy difference between NNET and Kriging, Kriging is easier to operate and insensitive to the number of points in the dataset.
- Significant CPU savings from ROM makes APECS more efficient and effective

- Gasifier ROM Integrated into steam cycle in GAMS - performs very well in process optimization. Excellent agreement with Fluent cases
- Results from ROM are more reliable than by Fluent (with larger residuals) - also avoids failure during iterations because of non-convergence of CFD simulator.

Remarks on Closed-loop Test

The closed-loop tests for yROM at Temperature, mass fraction of H_2S, H_2O, H_2 and CO show smaller differences comparing with the solutions of Fluent. While larger differences happened for CO_2 and CH_4. These are consistent with validation of ROM in Part I

Since Fluent model of gasifier used DPM The differences heavily depend on the performances of Fluent, i.e. the control residuals. The larger the residuals remain, the larger differences on CO_2 and CH_4 are observed. That is inherant from the limitation of the DPM.

yROM of Gasifer is powerful to integrate with flowsheets for process optimizations. It not only keep iterative optimization fast, but also guarantees computing smoothly while Fluent might failure to converge.

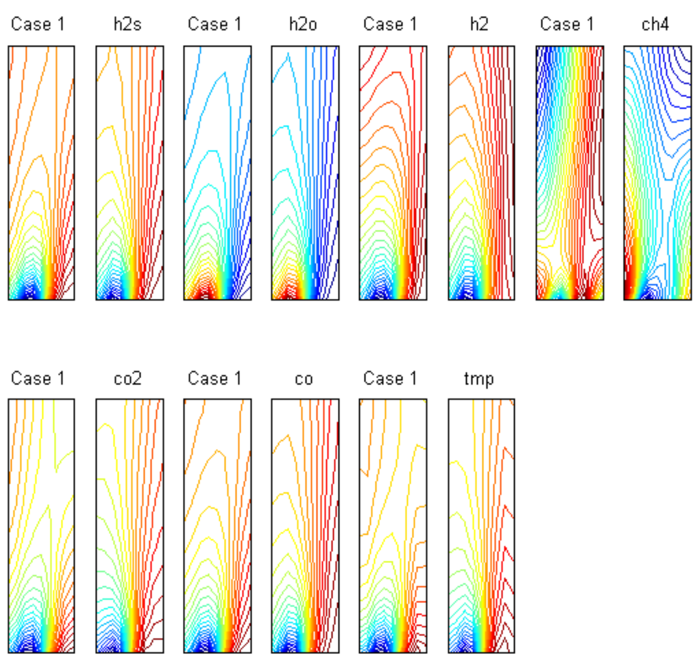
Summary

- **The methodology of ROM based on PCA takes full advantage of commercial packages and retains the complexities of CFD**
- **The methodology avoids the need to further manipulate complicated PDEs (unlike POD)**
- **The resulting ROMs are expected to remain valid over entire iterative simulation or optimization cycle**
- **Significant CPU time savings of ROM makes APECS more efficient and effective**

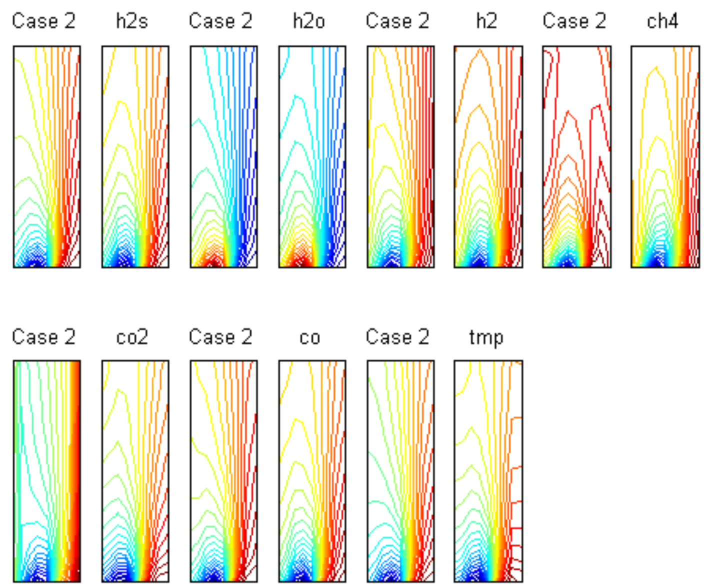
Future Work

- More ROMs will be developed for units such as
  - Gas turbine combustor
  - PSA
- Choose and build a platform in Aspen Plus for integration of more ROMs
- Convert ROMs into Equation-Oriented model (User3 or ACM) in protocols of Aspen Plus.
- Implement optimization with integrated Black-box
- More closed loop testing for new ROMs

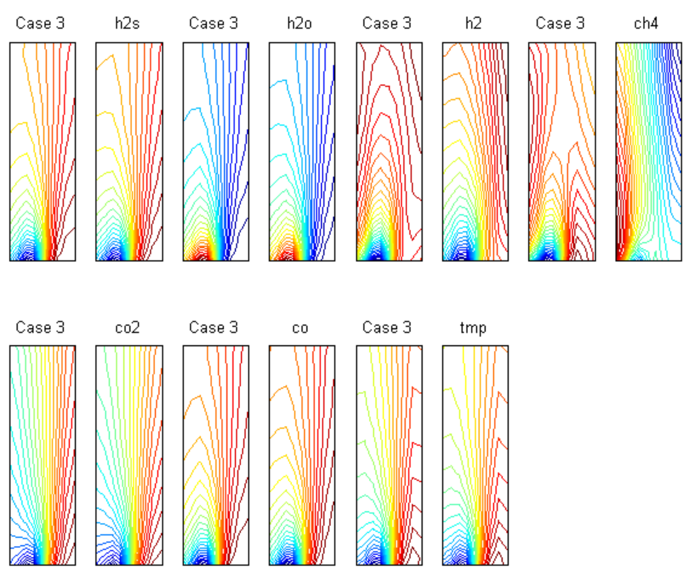
Closed Loop (1) for xROM



Closed Loop (2) for xROM



Closed Loop (3) for xROM



Closed Loop (4) for xROM